



A CFD Analysis of Hydrogen Leakage During On-Pad Purge in the ORION/ARES I Shared Volume

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Abstract

A common open volume is created by the stacking of the Orion vehicle onto the Ares I Upper Stage. Called the “Shared Volume”, both vehicles contribute to its gas, fluid, and thermal environment. One of these environments is related to hazardous hydrogen gas. While both vehicles use inert purge gas to mitigate any hazardous gas buildup, there are concerns that hydrogen gas may still accumulate and that the Ares I Hazardous Gas Detection System will not be sufficient for monitoring the integrated volume. This Computational Fluid Dynamics (CFD) analysis has been performed to examine these topics. Results of the analysis conclude that the Ares I Hazardous Gas Detection System will be able to sample the vent effluent containing the highest hydrogen concentrations. A second conclusion is that hydrogen does not accumulate under the Orion Service Module (SM) avionics ring as diffusion and purge flow mixing sufficiently dilute the hydrogen to safe concentrations. Finally the hydrogen concentrations within the Orion SM engine nozzle may slightly exceed the 1 percent volume fraction when the entire worst case maximum full leak is directed vertically into the engine nozzle.

Nomenclature

CFD	Computational Fluid Dynamics
cm	centimeter
cm ²	square centimeters
e	exponent
F	Fahrenheit
H ₂	hydrogen
in. ²	square inches
IU	Instrument Unit
K	Kelvin
kg/m ³	kilogram per cubic meter
kg/min	kilogram per minute
kg/s	kilogram per second
lb/ft ³	pounds per cubic foot
lbm/min	pounds mass per minute
scfm	standard cubic feet per minute
scim	standard cubic inches per minute
scmm	standard cubic meters per minute
SM	Service Module
T	temperature

1.0 Introduction and Objectives

Previously a CFD analysis had been performed on the shared Orion/Ares I volume in order to examine thermal effects and mixing. From this initial work, it became relatively easy to explore the hydrogen leakage topic. As with the previous CFD analytical work, this analysis utilizes the software FLUENT (ANSYS, Inc.) which has the ability to model the effects of different gas species.

Objectives of the CFD analysis are:

- **Objective 1.**—Determine if the Orion Service Module needs to implement a hazardous gas detection function at its vents.
- **Objective 2.**—Determine the interaction of the hydrogen gas with the purge flows in the shared volume and identify areas of potential hydrogen accumulation.
- **Objective 3.**—Determine if the concentration (by volume) of the hydrogen gas exceeds the safety margin of 1 percent volume fraction at any location (over a given time-period) in the shared volume.

2.0 CFD Model Development

This section describes the CFD model developed, the assumptions, and solution parameters to study the extent and concentration of hydrogen gas in the ORION/ARES shared volume.

2.1 Model Geometry

The geometry of interest is the “shared volume” between the Orion SM and Ares I IU. Figure 1 shows a cut-away view of the bounding surfaces of the shared volume as modeled with the FLUENT code. It is worth noting that most of the interior obstructions (e.g., solar arrays, antennae, avionics boxes, and piping/conduits) are not included in the model. Compared to the overall volumes, these items present a very small fraction of this volume and are not expected to significantly influence the gas flow paths or the gas velocity magnitudes for the purposes of this analysis.

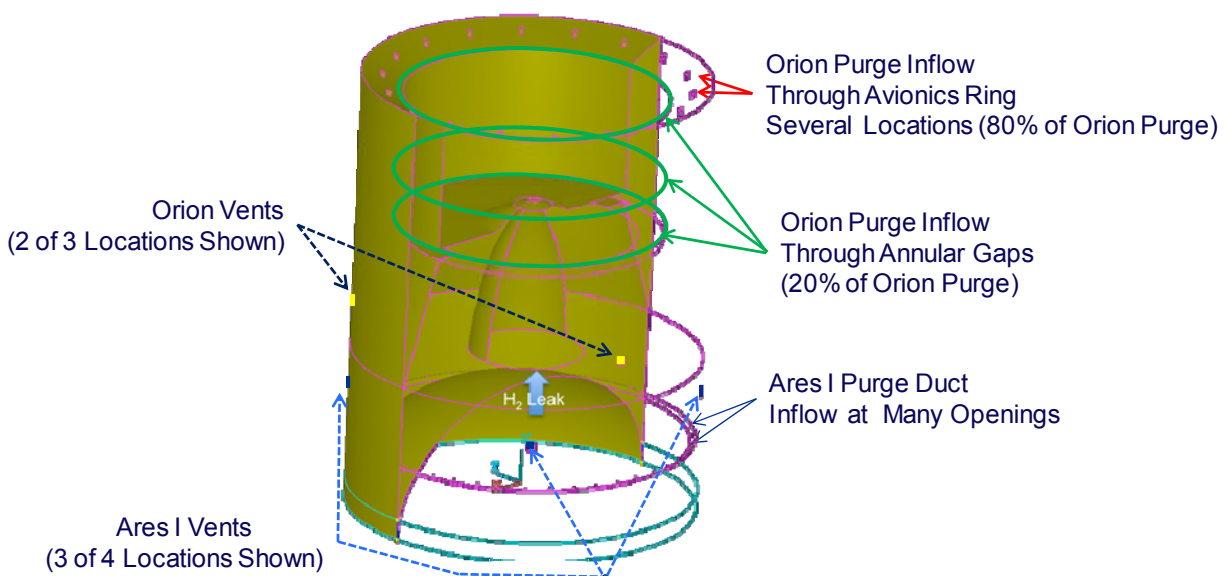


Figure 1.—Surface geometry for shared volume for SM/IU.

2.2 Assumptions

1. **Hydrogen Leak Location.**—Hydrogen will exist in the Liquid Hydrogen tank and internal to tubes/piping at the top of the tank. The geometry is shown graphically (but not to scale) in Figure 2. For the purpose of this analysis, the leak location is assumed to be around the valve and bolted flanges/fittings near the center of the tank. In the analytical model, the leak is modeled as an annular opening with total area of 0.2046 in.² (1.32 cm²) in the surface of the hydrogen tank. The area of this opening was chosen so as to provide the same order of inflow velocity as the surrounding purge flow.

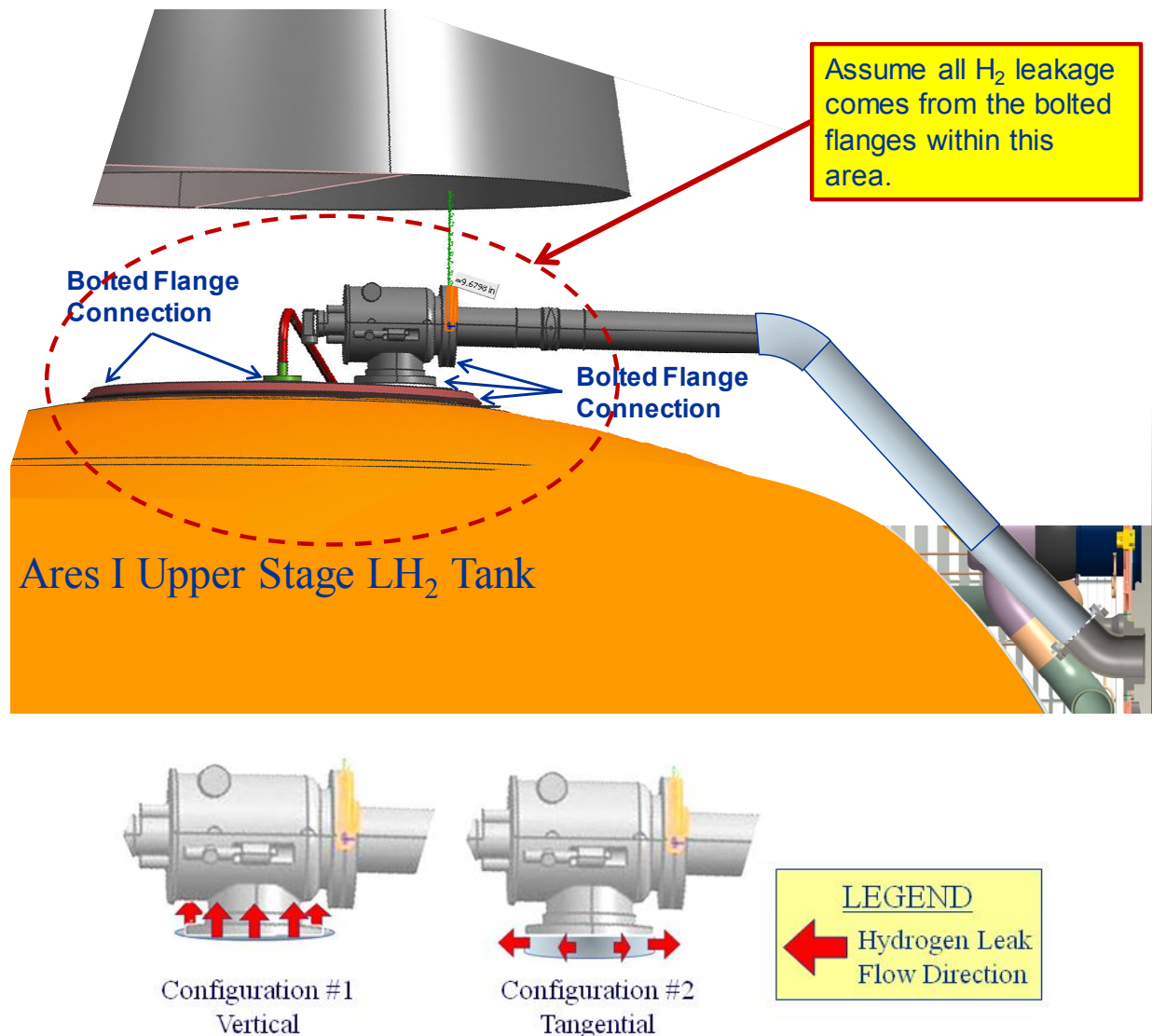


Figure 2.—General configuration used for hydrogen leakage.

2. **Hydrogen Leak Amount.**—The nominal leak rate used for this analysis is 1400 scim. The source of this value is Table 14 of CxP72034B, Ares I Systems Requirements Document. It is considered the leakage limit during propellant loading and first stage flight operations for hydrogen leakage into the Instrument Unit.
3. **Hydrogen Leak Direction Orientation.**—Since the actual mechanism of the hydrogen leak is extremely difficult to characterize, the nature of the leak was deemed to be bounded by two configurations for the inflow of the hydrogen into the shared volume.
 - **Configuration 1.**—Hydrogen flows in a direction normal to the top most point of the tank and vertically into the engine nozzle. This would represent the worst case for hydrogen accumulation within the engine nozzle.
 - **Configuration 2.**—Hydrogen flows in a direction tangential to the top surface of the tank in a direction normal to the axis of the vehicle. This is thought to represent the most likely case for hydrogen spreading into the SM's annular space between the SM radiators and the fairings.

The real-world nature of the hydrogen leak is somewhere in between these two configurations modeled by the CFD analysis.

4. **Purge Flowrates.**—Nominal nitrogen purge flowrates are 150 lbm/min (68.04 kg/min) through the Ares I IU purge duct and 100 lbm/min (45.36 kg/min) through the Orion SM. For this analysis, the general purge flow distribution for Orion uses an 80 and 20 percent split (Avionics Ring openings and Propulsion System Assembly openings). Final Orion purge flow split will likely be significantly different than these values, but since the total flowrate remains the same with all Orion openings into the shared volume above the Orion-Ares I gap and the flow in Ares is the dominating flow, it is not expected to have any significant impact on the results. The purge flowrates for both vehicles will operate over a range of values and will not be expected to operate at the nominal flowrate at all times. For example, purge flowrates are expected to vary from 90 lbm/min to 100 lbm/min (40.82 to 45.36 kg/min) for Orion. A conservative analysis would target the low end of this range. However, since a separate computer run has already been performed using a 10-times increase in hydrogen leak rate, it was decided to not perform another computer run for the lower purge flow as its results would be enveloped by this larger relative change in hydrogen flow rate.
5. **Purge Temperatures.**—Thermal variations in the purge flow temperature and environmental heating is not included in this analysis. Again, these are perceived to be an insignificant influence on the hydrogen gas motion. A secondary analysis with warm/cold inflow temperature for the Hydrogen gas shows that this assumption is indeed conservative.
6. **No Other Gas Inflows.**—Inflow of external air or leakage of any other fluid into the shared volume is considered as zero. This assumption is expected to produce a conservative result as any further fluid constituents would only serve to lower the hydrogen concentration values.

2.3 Input Flow Conditions

The flow-rates for the various fluids entering the shared volume are:

- Purge flow of nitrogen through SM inlets = 100 lbm/min (45.36 kg/min) or 1356 scfm (38.40 scmm)
- Purge flow of nitrogen through IU inlets = 150 lbm/min (68.04 kg/min) or 2034 scfm (57.60 scmm)
- Hydrogen maximum leak flow rate = 1400 scim or 0.81 scfm (0.0229 scmm) which equates to approximately **0.004237** lbm/min (**0.001922** kg/min)
- Based on hydrogen density = 0.005231 lbm/ft³ (**0.0838** kg/m³) using standard conditions of 67.4 °F (293 K) at standard atmospheric pressure

Note: The volumetric flow rate of the nitrogen purge gas at 3390 scfm (96.0 scmm) is more than three orders of magnitude greater than the specified maximum hydrogen leak rate of 0.81 scfm (0.0229 scmm).

Since the scope of the current analysis did not permit a detailed modeling of the heat-transfer on the surface of the hydrogen tank, multiple cases of this analysis were performed to evaluate the effect of the leaking gas's temperature. For the purpose of this analysis, the hydrogen properties used as CFD code inputs for the two temperature conditions are summarized in the following table.

TABLE 1.—HYDROGEN PROPERTIES

Characteristic	Cold hydrogen, 100 K (−280 °F)	Warm hydrogen, 300 K (80 °F)	Units
Density	0.2456	0.08188	kg/m ³
	0.01533	0.005112	lb/ft ³
Volumetric flowrate	0.000691	0.002040	m ³ /min
	0.024409	0.072047	ft ³ /min
Mass flowrate	187.5	188.2	kg/min
	413.37	414.90	lbm/min
Hydrogen mole fraction	2.297e-4	2.306e-4	-----

2.4 FLUENT Solution Parameters

The commercial code FLUENT was used as the CFD tool to perform the computations for the geometry and flow conditions described above. A summary of the primary parameters for the CFD solution are listed below:

- 1.4 million nodes
- Green-Gauss node-based solution, incompressible flow formulation
- SIMPLE pressure-velocity coupling, **steady-state** solution
- Realizable k-epsilon turbulence model
- Four-species mixture model (non-reacting)
- SM Purge Flow is 95 percent nitrogen, 5 percent oxygen (oxygen is used as a tracking species for analytical purposes)
- IU Purge Flow is 95 percent nitrogen, 5 percent methane (methane is used as a tracking species for analytical purposes)
- Second-order accurate spatial discretization for all equations
- Solve for continuity, momentum, energy, k-epsilon and species
- Fixed mass-flow rate at all inflow boundaries (nitrogen purge and H₂ inflow as specified at given temperature)

- SM Avionics Ring, 18 holes at 3.0 in. (7.62 cm) diameter = 83.6 lbm/min (37.92 kg/min)
- SM eyelid = 0.0873 lbm/min (0.0396 kg/min)
- SM Radiator Gaps: Top/Bottom = 6.627 lbm/min (3.006 kg/min) each;
Mid = 2.831 lbm/min (1.284 kg/min)
 - The gaps between the radiator panels are modeled as circumferential gaps; one at the top, one in the middle, and one at the bottom. These circle the outer surface of the SM as rings.
- IU holes = 67.98 kg/min flowing through 44 holes at 0.75 in. (1.905 cm) diameter
- Fixed back-pressure at all outflow vents (SM and IU)

3.0 FLUENT Results

3.1 Vertical Injection of Hydrogen

The FLUENT code was run for configuration 1 in which H₂ leaking into the shared volume at 80 °F (300 K) is in a direction aligned with the long axis of the vehicle. As discussed in Section 2.1, this configuration represents the worst case scenario for H₂ accumulation in the SM engine nozzle. A cold hydrogen gas case was not run in this vertical configuration as it would not yield worst case results due to the cold gas tendency to go downward first and then spread outward causing some of the gas to go beyond the engine nozzle opening. A summary of the primary CFD results is given below:

- Excellent convergence for mass-flow rate imbalance of purge flows.
- Difference between inflow and outflow is approximately 1.0e-6 kg/s (roughly 0.00005 percent)
- Convergence of species mass-concentration for H₂ “stalls” near 1.0e-4 (see Fig. 3)
 - Possibly “unsteady” flow effects in primary flow (IU cavity)

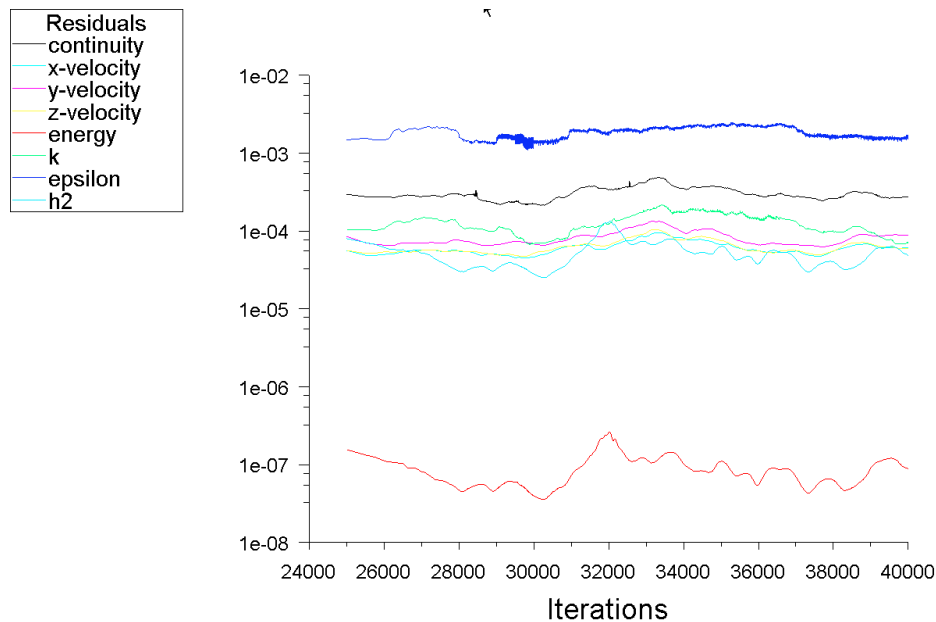


Figure 3.—Convergence history for vertical injection.

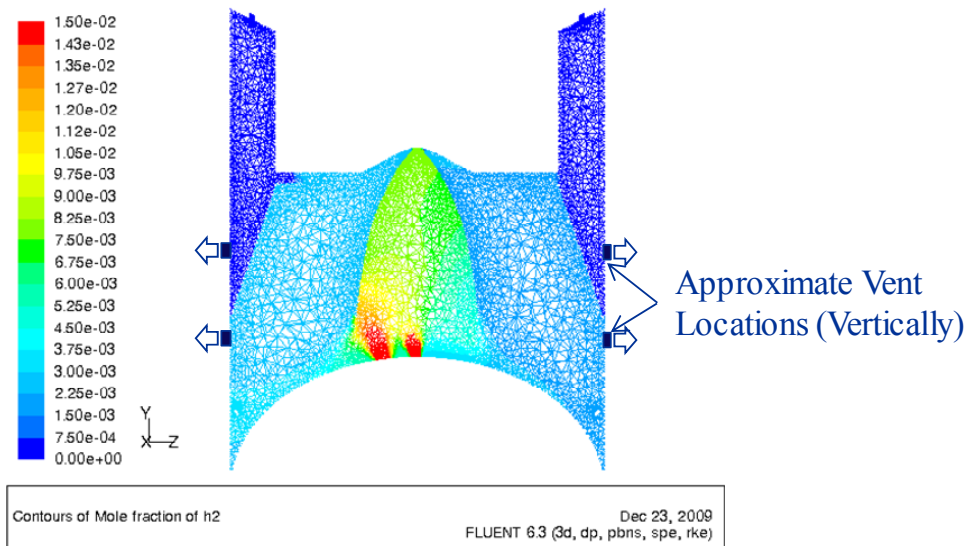


Figure 4.—Contours of mole fraction of Hydrogen in shared volume.

Figure 4 shows contours of mole fraction of the leaked hydrogen gas in a cross-sectional plane of the shared volume. The effect of the vertical injection is that most of the hydrogen accumulates in the engine nozzle, and a very low concentration of H_2 is seen in the IU cavity. A small fraction of the H_2 gas makes its way past the SM/IU gap and there is almost no H_2 in the annular area between the SM radiator and the vehicle outer surface.

To help demonstrate that the analysis is properly accounting for the hydrogen, the exiting hydrogen mole fraction was compared to the incoming hydrogen mole fraction. For a steady state condition where purge flowrates and hydrogen leakage rates are constant, the values would be expected to be nearly identical. In this case, the circulating flows create a condition where a true steady state cannot be analytically achieved, causing the mole fraction values to be not identical. Yet, the values still provide insight into how well the analysis is accounting for the hydrogen molecules and where they are flowing. For this vertical injection case, the average mole fractions of H_2 exiting the three SM and four IU vents were computed as $0.665e-4$ and $3.56e-4$, respectively for an overall average of $2.32e-4$ for all seven vents (compares favorably to the $2.306e-4$ warm case input value). Note: For these conditions (approximately ambient temperatures and pressure), the mole fraction and the volume fraction can be considered as the same numerical value. The maximum concentration of H_2 in the SM engine nozzle is around the 1 percent level (yellow to orange colors) except in the area near the leak where H_2 levels go above the 1 percent safety limit—however, this is to be expected in the vicinity of the leak.

Figure 5 shows velocity vectors in a cross-sectional plane of the shared volume. The vectors are scaled by the velocity magnitude in the flow. The IU cavities between the conical adapter and the SM engine nozzle show very strong recirculation of the purge flow. The area enclosed by the engine nozzle also shows some weak vortical structures around the H_2 injection location.

Previous CFD analysis has shown that a degree of mixing occurs between the SM and IU purge gases within the shared volume. To help visualize this mixing, particle tracing was performed to follow the route of various particles through the shared volume. Figure 6 shows particle traces representing the path traversed by a few particles that enter the domain through the SM avionics ring vents. While none of these particular particle traces actually exited through the IU vents, some did enter the IU volume. It can be concluded that some of the purge flow that enters the domain via the SM will eventually exit the domain via the IU vents. For this analytical run, total flow rate at the IU and SM vents was computed as 146.94 and 103.06 lbm/min (66.65 and 46.75 kg/min), respectively. This agrees very well with the incoming flow-rates of 150 and 100 lbm/min (68.04 and 45.36 kg/min) at the IU and SM purge inlets, respectively.

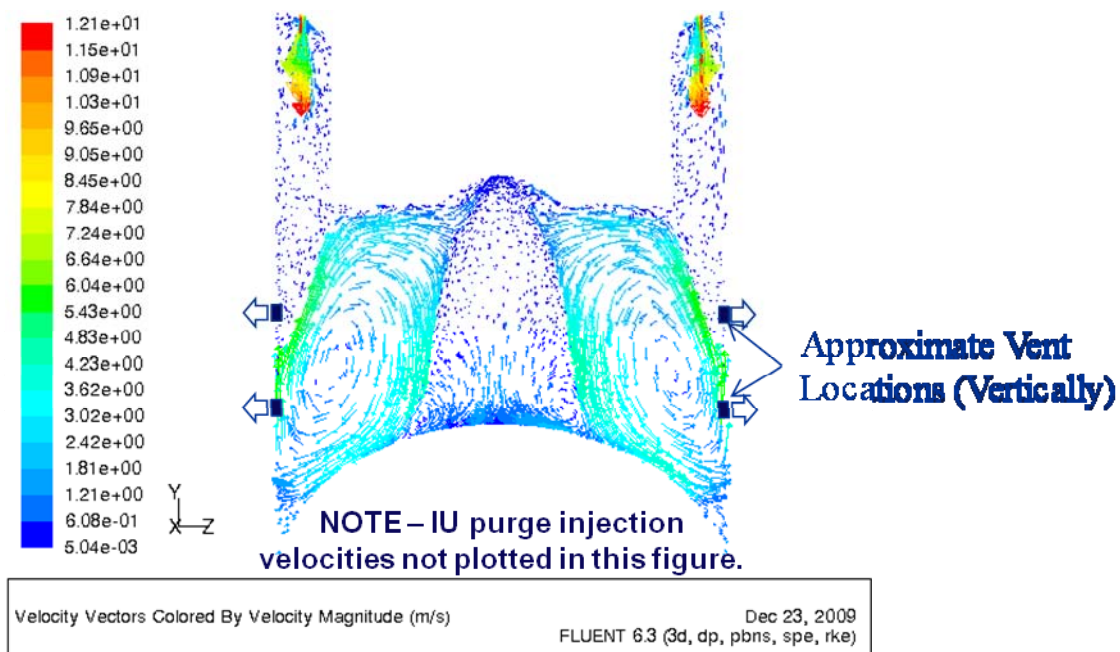


Figure 5.—Velocity vectors (colored by velocity magnitude) in shared volume.

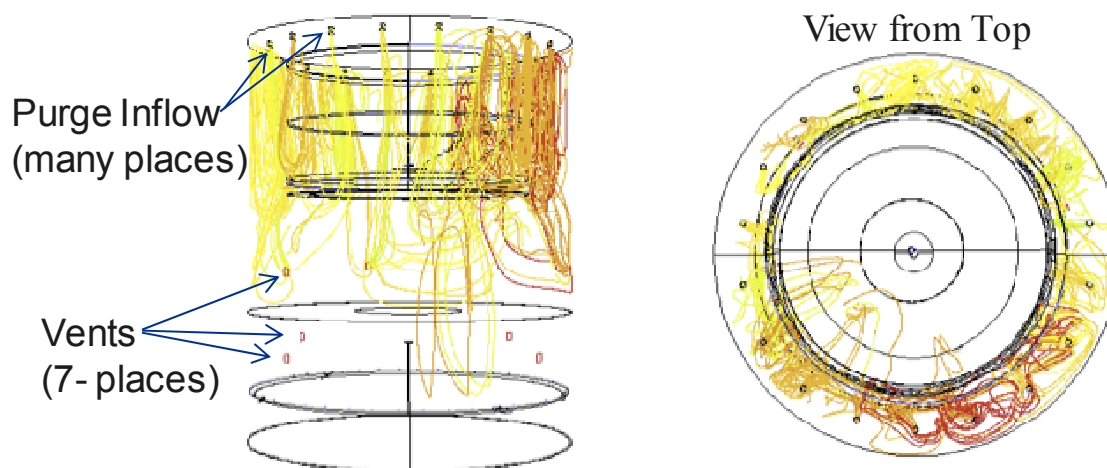


Figure 6.—Particle traces representing SM avionics ring flow into the shared volume.

3.2 Tangential Injection of Hydrogen

Simulating the hydrogen leak at a tangential direction was used for three cases. The tangential “orifice” was located at radius = 1.8 in. (4.572 cm) with height = 0.01809 in. (0.04595 cm) for an area of 0.2046 in.² (1.32 cm²) which is the same area as the vertical injection case. First case is the base case which is used to compare with the vertical leak direction in Section 3.1. The second case explores the temperature effect of the leaking hydrogen gas by assuming it is cold and consequently at a greater density (less buoyant). The third case is used to examine the situation of a hydrogen leak rate that far exceeds the specified maximum limit.

3.2.1 Baseline Case

The FLUENT code was run for configuration 2 where the H₂ is leaking into the shared volume in a plane normal to the long axis of the vehicle (tangential to the topmost point of the H₂ tank). As discussed in Section 2.2 assumption 3, this configuration represents the scenario for maximum H₂ spreading into the SM portion of the shared volume. Results show the overall exit flow at the IU and SM vents to be 146.9 and 103.1 lbm/min (66.63 and 46.77 kg/min), respectively. Now checking the flow of hydrogen, the average mole fraction of H₂ exiting the (three) SM and (four) IU vents was 1.113e-4 (note this is 67 percent higher than “vertical” injection) and 3.216e-4 (10 percent lower than “vertical”), respectively, for an overall average of 2.315e-4 exiting the seven vents (incoming value is 2.306e-4). This result confirms the horizontal leak mechanism as being the worse case for hydrogen reaching into the SM portion of the shared volume.

Figure 7 illustrates the variation of H₂ concentration in the computed volume over time which occurs due to the oscillating nature of the purge flow in the IU cavity. The set of six contour plots shows that a quasi-steady solution may be assumed between 35000 and 45000 time-steps. The results at 35000 steps show that there is some spread of H₂ into the IU cavity. However, as the

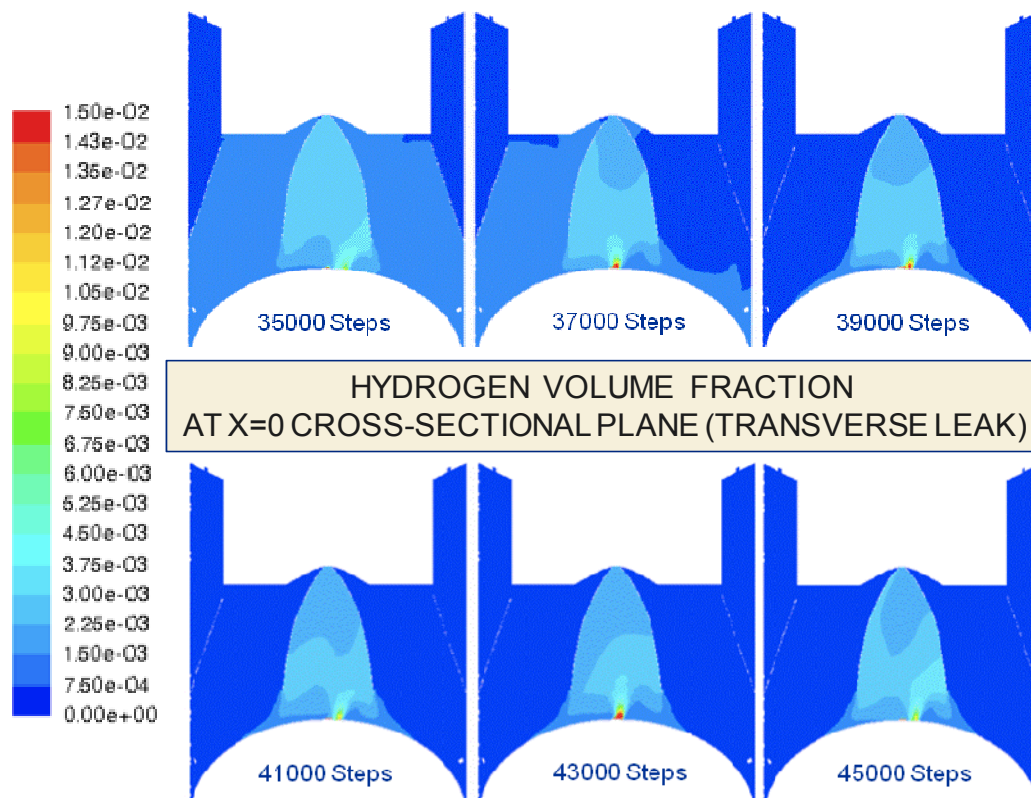


Figure 7.—Variation of hydrogen concentration over time at T = 80 °F (300 K).

solution approaches a quasi-steady state at 45000 steps, the H_2 concentration in the cavity drops to trace amounts. The maximum volume fraction of H_2 at the quasi-steady state (45000 steps) is well below the safety margin of 1 percent volume fraction of H_2 .

It may also be noted that there does not seem to be any significant qualitative differences in the spread of H_2 into the SM shared volume due to either tangential injection or vertical injection (compare Fig. 7 with Fig. 4 in Section 3.1). This is possibly because the strong vortical flows (shown in Fig. 5) created by the comparatively high flow rates of the IU and SM purge flows tend to dominate the overall flow pattern in the regions outside of the SM engine nozzle.

3.2.2 Off Design Case—Cold Hydrogen Leak

In order to study the effect of variation in temperature of the leaking H_2 , an off-design case representing “cold” flow was simulated with the FLUENT code. The H_2 gas was injected “tangentially” into the shared volume at a temperature of -280°F (100 K). The leak simulation was initiated from a converged solution representing the baseline purge flow (without any leak). Figure 8 shows a time-history of the H_2 mole-fractions for the cold flow case. For this case, the heavier H_2 spreads more slowly into the volume and shows lower concentrations of H_2 in the SM engine nozzle region when compared to the warm case (see Fig. 7). The overall exit mass flowrate at the IU and SM vents is 146.5 and 103.5 lbm/min (66.445 and 46.95 kg/min), respectively. Checking where the hydrogen is flowing, the average mole fractions of H_2 exiting the (three) SM and (four) IU vents were $6.92\text{e-}5$ (38 percent lower than “baseline”) and $3.55\text{e-}4$ (10 percent higher than “baseline”), respectively. The overall average hydrogen mole fraction exiting all seven vents is $2.325\text{e-}4$ while the incoming value is $2.306\text{e-}4$.

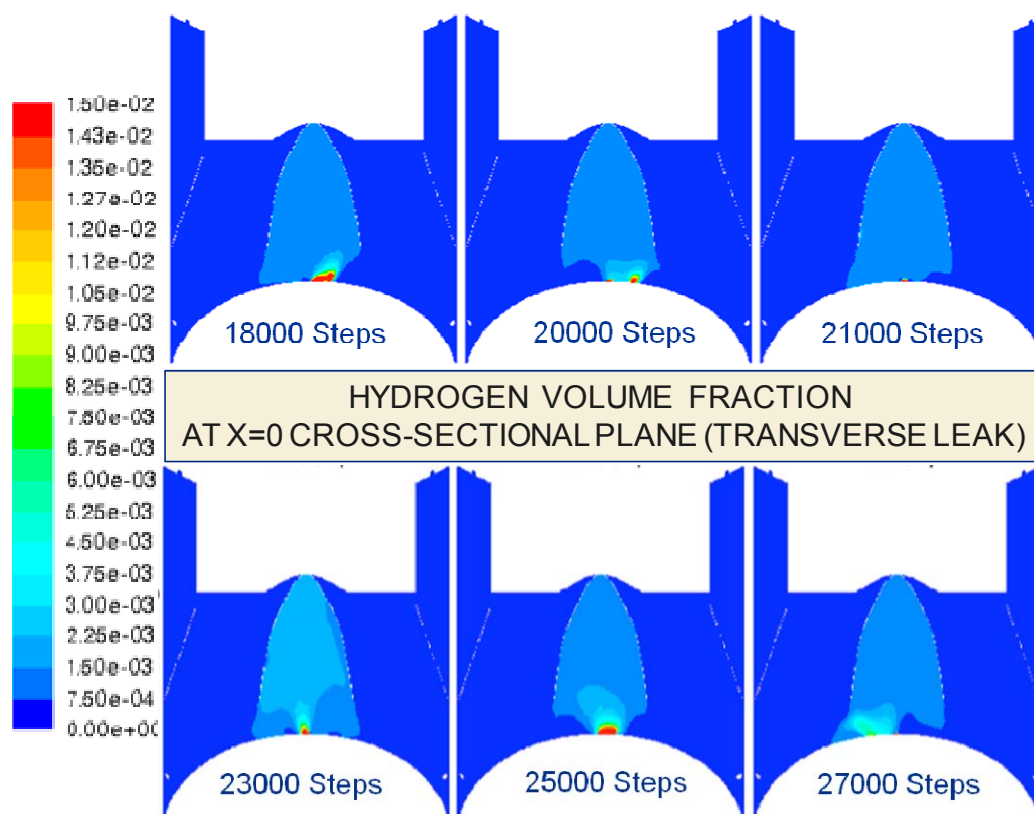


Figure 8.—Variation of hydrogen concentration over time at $T = -280^\circ\text{F}$ ($T = 100\text{ K}$).

3.2.3 Off Design Case—10x Hydrogen Leak Flow Rate

As observed in Sections 3.1 and 3.2.1, the maximum concentration (by volume) of H_2 in the shared volume was computed to be well below the safety limit of 1 percent concentration of hydrogen by volume for the nominal maximum H_2 flow rate of 0.81 scfm (0.0229 scmm). An off-design case was conceived with a significantly increased hydrogen flow-rate of 8.1 scfm (0.229 scmm), which is an order of magnitude increase in maximum leak rate, to determine if the H_2 concentration would perhaps exceed the 1 percent safety limit in the shared volume. This is more an examination of the design's robustness than an actual case. The results would also envelope any impacts from operating at the low range of the nitrogen purge flowrates.

Figure 9 shows the variation of H_2 concentration in the computed volume for the 10 times leak flow-rate. The results show that there is considerably more H_2 in the IU cavity for this case with some H_2 making its way into the SM annular region. While the volume fraction of H_2 exceeds the 1 percent margin within the SM engine nozzle, the remaining volumes of the IU and SM have hydrogen concentration values still under the 1 percent limit.

It is worth noting that an increased hydrogen concentration value will be detected at the vents by the Hazardous Gas Detection System, yet still be under the 1 percent limit. The SM engine nozzle is still under the 4 percent concentration value for becoming an actual hazard and the environment is still nitrogen purged to prevent a flammable mixture from developing (assumes there is no simultaneous oxygen leak). The average mole fraction of H_2 exiting the three SM and four IU vents were $0.765e-3$ and $3.4e-3$, respectively, for an overall average of $2.27e-3$ for all seven vents (compared to the input H_2 mole-fraction of $2.306e-3$).

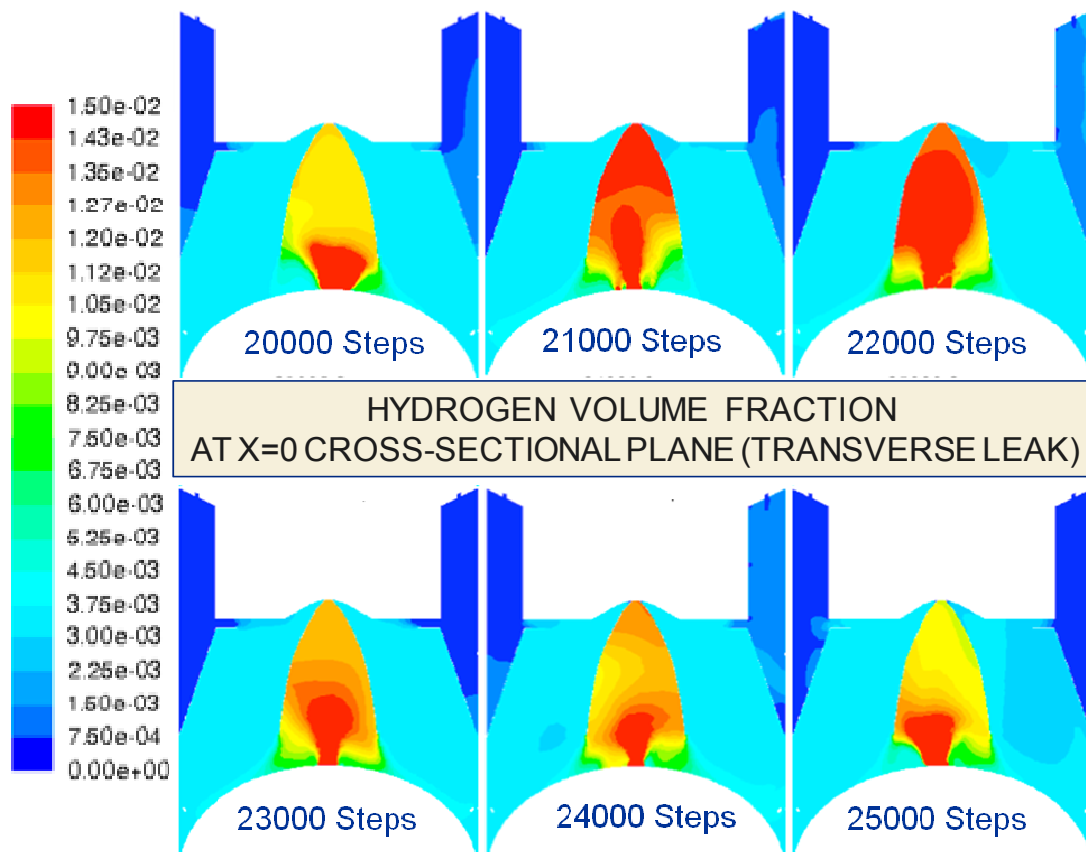


Figure 9.—Variation of Hydrogen concentration over time, 10 times leak rate.

4.0 Conclusions and Recommendations

A CFD simulation of H₂ leakage into the Orion/Ares shared volume has been completed with the FLUENT code. The entry of the leaking gas into the shared volume can be successfully “bounded” by assuming that the H₂ flows either horizontally along the vehicle axis or normal to the vehicle’s long axis. At the nominal designed max hydrogen leak rate of 1400 scim (0.0229 scmm), the concentration of the H₂ gas does not exceed the safety margin of 1 percent accumulation (by volume) at any location in the shared volume. A CFD simulation with an off-design leak flow-rate using 10 times the maximum specified flowrate, does show that the safety-margin could be exceeded within the SM engine nozzle, but not elsewhere in the shared volume.

The CFD modeling approach developed during this work provides reasonable insight into the physical behavior of leaking H₂ in the presence of background purge flow. In the absence of any experimental data, the modeling approach can be used as a viable independent validation and verification tool to perform detailed parametric studies for similar configurations or flow conditions.

Objective 1.—Determine if the Orion Service Module needs to implement a hazardous gas detection function at its vents.

TABLE 2.—SUMMARY
[Hydrogen Concentration (volume fraction) exiting vehicle vents.]

	Vertical	Tangential		
	Baseline, percent	Baseline, percent	Cold, percent	10X Leak, percent
Orion SM vents	0.0068	0.0113	0.0070	0.0770
Ares IU vents	0.036	0.0327	0.0361	0.3461

Results show that in all cases the concentration of hydrogen exiting the Ares IU vents is greater than the concentration exiting the SM vents. Therefore, it can be concluded that the Ares IU Hazardous Gas Detection System will be monitoring the worse case and there is no need to add monitoring capability at the Orion SM vents.

Objective 2.—Determine the interaction of the hydrogen gas with the purge flows in the shared volume and identify areas of potential hydrogen accumulation.

Hydrogen diffuses rapidly and is entrained in the purge flows as they find their way to the exit vents. Hydrogen concentrations can build up in the SM engine nozzle to a level higher than the rest of the shared volume, especially if the leak gets directed into the engine nozzle. By running the off-nominal case of a hydrogen leak rate ten times the maximum specified rate, it was determined that the concentration in the SM engine nozzle can exceed the 1 percent limit, but does remain below the 4 percent hazardous value. This would indicate that the SM engine nozzle can be considered a potential location for hydrogen accumulation during off-nominal conditions.

Objective 3.—Determine if the concentration (by volume) of the hydrogen gas exceeds the safety margin of 1 percent volume fraction at any location (over a given time-period) in the shared volume.

Under the worse case, the hydrogen concentration in the SM engine nozzle may slightly exceed the 1 percent volume fraction safety limit in the vicinity of a directed hydrogen leak. However, it is concluded that under the nominal maximum hydrogen leak rate, there will be no accumulation of hydrogen that would violate the safety limit at any other location beyond the vicinity of the leak source. It is recommended that the analysis be re-performed as the designs evolve in order to assess the need for development of mitigation strategies.

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14. ABSTRACT A common open volume is created by the stacking of the Orion vehicle onto the Ares I Upper Stage. Called the "Shared Volume", both vehicles contribute to its gas, fluid, and thermal environment. One of these environments is related to hazardous hydrogen gas. While both vehicles use inert purge gas to mitigate any hazardous gas buildup, there are concerns that hydrogen gas may still accumulate and that the Ares I Hazardous Gas Detection System will not be sufficient for monitoring the integrated volume. This Computational Fluid Dynamics (CFD) analysis has been performed to examine these topics. Results of the analysis conclude that the Ares I Hazardous Gas Detection System will be able to sample the vent effluent containing the highest hydrogen concentrations. A second conclusion is that hydrogen does not accumulate under the Orion Service Module (SM) avionics ring as diffusion and purge flow mixing sufficiently dilute the hydrogen to safe concentrations. Finally the hydrogen concentrations within the Orion SM engine nozzle may slightly exceed the 1 percent volume fraction when the entire worst case maximum full leak is directed vertically into the engine nozzle.					
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